The DOE Center of Excellence for the Synthesis and Processing of Advanced Materials (CSP)

Overview

The DOE Center of Excellence for the Synthesis and Processing of Advanced Materials (CSP) is a distributed center for promoting coordinated, cooperative research partnerships related to the synthesis and processing of advanced materials. It was established by DOE's Division of Materials Sciences and Engineering, Office of Basic Energy Sciences and the DOE Laboratories in recognition of the enabling role of materials synthesis and processing to numerous fabrication- and manufacturing-intensive technologies. The participants include investigators from 12 DOE national laboratories, universities and the private sector. The Center has a technology perspective which is provided by a Technology Steering Group.

The current emphasis of the Center is on eight focused multilaboratory projects which draw on the complementary strengths of the member institutions in their ongoing research programs. These eight projects were selected on the basis of the following criteria: (1) scientific excellence, (2) clear relationship to energy technologies, (3) involvement of several laboratories, (4) existing or potential partnerships with DOE Technologies-funded programs, and (5) existing or potential "in-kind" partnerships with industry.

The eight projects are:

- Design and Synthesis of Ultrahigh-Temperature Intermetallics
- Isolated and Collective Phenomena in Nanocomposite Magnets
- Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors
- The Science of Localized Corrosion
- Smart Structures Based on Electroactive Polymers
- Nanoscale Phenomena in Perovskite Thin Films
- Granular Flow and Kinetics
- Synthesis and Processing of Carbon-Based Nanostructured Materials

The member laboratories of the Center are: Ames Laboratory (Ames), Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Idaho National Engineering and Environmental Laboratory (INEEL), University of Illinois Frederick Seitz Materials Research Laboratory (UI/MRL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), National Renewable Energy Laboratory (NREL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL). The Center also includes appropriate university grant research and some industry participation.

Objective

The overall objective of the Center is,

"To enhance the science and engineering of materials synthesis and processing in order to meet the programmatic needs of the Department of Energy and to facilitate the technological exploitation of materials".

Synthesis and processing (S&P) are those essential elements of materials science and engineering (MS&E) that deal with (1) the assembly of atoms or molecules to form materials, (2) the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and (3) the development of processes to produce materials for specific applications. Clearly, S&P represent a large area of MS&E that spans the range from fundamental research to technology. The goal of basic research in this area ranges from the creation of new materials and the improvement of the properties of known materials, to the understanding of such phenomena as diffusion, crystal growth, sintering, phase transitions, etc., in relation to S&P. On the applied side, the goal of S&P is to translate scientific results into useful materials by developing processes capable of producing high quality, cost-effective products.

Materials and Processes Focus of the Center

The current emphasis of the Center is on the eight projects cited above.

Each of the projects is coordinated by an appropriate representative from one of the participating institutions. The overall Center coordinator is:

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A brief description of each project follows:

Design and Synthesis of Ultrahigh-Temperature Intermetallics

Participating Labs:	Ames, ANL, INEL, LANL, LBNL, LLNL, UI/MRL, ORNL, and SNL/CA		
Coordinators:	R. Judkins (ORNL)	and	R. B. Thompson (Ames)
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This project has the ultimate goal to develop scientific principles to design new-generation intermetallic alloys for structural applications at temperatures at and above 1400°C. The initial thrust is on Mo_5Si_3-base alloys which possess outstanding high-temperature strength and oxidation resistance (when alloyed with boron). The broad objective is to generate the knowledge required to establish a scientific basis for the processing and design of transition-metal silicides with improved mechanical and metallurgical properties at ambient and elevated temperatures.

The project is organized into three major tasks as follows: (1) first-principles calculations, atomistic simulations, and mechanical modeling; (2) experimental study and correlation of structure and properties; and (3) innovative materials processing and fabrication of high-purity materials.

The project builds on base programs funded by BES at all participating institutions; by Fossil Energy Advanced Research and Technology (AR&TD) programs at ANL, INEL, and ORNL; and by Energy Efficiency Advanced Industrial Materials (AIM) programs at Ames Laboratory, LANL, and ORNL.

Isolated and Collective Phenomena in Nanocomposite Magnets

Participating Labs:	Ames, ANL, BNL, INEEL, UI/MRL, LANL, LBNL, LLNL, ORNL, and SNL
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The objective of this project is to develop improved understanding of magnetic properties and improved magnetic materials using nanoscale mixtures of hard magnets, soft magnets and non-magnetic materials. The program will address the behavior of isolated, well-defined magnetic particles; the assembly of these into controlled structures; and the investigation of bulk materials with simple, defined microstructures.

The project has three tasks: (1) Synthesis and investigation of isolated magnetic nanoparticles; (2) synthesis and investigation of collective behavior in materials with defined microstructures; and (3) modeling and simulation of nanoscale magnets.

The project has both university and industrial collaborators. Currently industrial collaborations are with Magnequench International, Rhodia, IBM, Motorola, IAP Inc. and Fujitsu. Current university collaborators include the University of Utah, University of Birmingham, Michigan Technological University, University of California-San Diego, Carnegie Mellon, Lehigh University, and the University of Nebraska.

Controlled Defect Structures in Rare-Earth-Ba-Cu-O Cuprate Superconductors

Participating Labs:	Ames, ANL, BNL, LANL, SNL, and ORNL
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The objective of this project is to provide an integrated scientific understanding of lattice defects and their nanoscale structure in the family of rare-earth cuprates with the “123” structure, $REBa_2Cu_3O_2$, their relationship to the various methods of synthesis and processing of both coated conductors and single-domain monoliths, and their relation to the resulting superconducting properties.

The project consists of four tasks: (1) specimen fabrication by state-of-the-art methods; (2) structural and chemical characterization using advanced and specialized methods of TEM; (3) electromagnetic characterization by transport magneto-optical and local probe measurements; and (4) theoretical modeling, including modeling of electromagnetic and flux-pinning properties of defects.

The project includes groups funded by BES (ANL, Ames), groups funded by the EE Superconductivity Program for Electric Systems (LANL, SNL), and groups funded by both (BNL, ORNL). The participating groups have strong connections, including CRADAs, with the principal corporations involved in the development and manufacture of conductors and monoliths, American Superconductor Corporation, Oxford Superconducting Technology, Intermagnetics General Corporation, and Superconductive Components, Inc., among others. Also members of the participating groups have strong collaborations with several universities with active applied superconductivity programs (Wisconsin, Northwestern, Illinois, Houston, et al.).

The Science of Localized Corrosion

Participating Labs:	Ames, BNL, LLNL, PNNL, SNL/NM, UI/MRL, Ohio State University, University of Utah, and University of Virginia
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The objective of this project is to advance our fundamental understanding of localized corrosion of aluminum materials to permit accurate life predictions and intelligent designs. We will generate a new and deeper understanding of the mechanisms leading to the initiation, propagation, and cessation of localized corrosion of aluminum and its alloys. Localized corrosion can be broken into several stages: precursors to electrochemical attack, the initiation of localized corrosion, the propagation of a localized corrosion site, and, in some cases, its cessation. Within each stage, there may be several relevant contributing factors, including: properties of the passive oxide layer and its outer surface, metallurgical factors, and influence of the environment.

The project consists of the following three tasks: (1) oxide structure and chemistry, (2) metallurgical factors, and (3) localized chemistry and electrochemistry.

The research in this project is relevant to several programs and needs in DOE Technologies, including the EE/Office of Transportation Technologies, DP/Enhanced Surveillance Program Office, DP/Office of Defense Sciences, and the Office of Civilian Radioactive Waste Management/Monitored Geological Repository Program. These Offices directly fund work in localized corrosion of aluminum materials (or, for OCRWM, other passive metals) at the participating laboratories. As active partners we have the Naval Research Laboratory, Alcoa, Ford Motor Company, and Lucent Technologies. These partners have ongoing research to address the issues in localized corrosion of aluminum that are pertinent to their applications.

Smart Structures Based on Electroactive Polymers

Participating Labs:	Ames, ANL, BNL, UI/MRL, INEEL, LBNL, LLNL, ORNL, PNNL, SNL/NM
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This project develops a framework for the rational design of self-assembled nanostructured block copolymers that offer significant advantages over conventional materials for active regulation of transport phenomena. Some examples include: optical and thermo-optical switches for use in smart paints or in color-converting clothing; ion-selective membranes for battery and fuel cell applications; intellomeres to promote self-healing and repair of composite structures; and thermally driven phase change material for smart insulation applications. Such examples seem particularly attractive both to the more applications oriented DOE Program Offices and the commercial sector with whom this project seeks to establish alliances. In order to realize such advanced materials, a multi-disciplinary program with a strong fundamental science underpinning is mandated. The project consists of four tasks.

The first task involves modeling properties at the molecular level. The goal here is to determine which chemical groups on a segment comprising a block and which molecular conformations associated with that segment promote the property of interest. For example, maximize nonlinear optical activity in a conjugated multi-aromatic ring system, the extent of conjugation, and twist angle between adjacent rings are important parameters.

In the second task, molecular architecture modeling, the interaction energies developed in the first task will be used to predict what structures likely will self-assemble for particular segment lengths, and polymer molecular weights. Conversely, simulated interaction energies can be used to guide the synthesis of new polymers.

The third task involves the development of synthesis and processing methods to achieve a targeted nanoarchitecture. This task is not constrained to the synthesis of only organic systems. N-block copolymers also will be prepared that include inorganic polymers (siloxanes, phosphazenes, ...) or mixed organic/inorganic moieties. A fourth task will involve structural determination and properties measurements of the synthesized n-block copolymers. Experimental results will be used to validate modeling predictions, modify modeling protocols, and further refine processing methods.

Nanoscale Phenomena in Perovskite Thin Films

Participating Labs:	ANL, LANL, ORNL, SNL/NM, Northwestern U., U. North Carolina, U. Maryland, U. Florida, N. Illinois	
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This project has two inter-related objectives with many team members participating in both.

Objective 1: Develop the scientific basis for controlling nucleation, growth, and strain in perovskite thin films. Critical issues are control of interface properties at the atomic scale, control of microstructure and film orientation, and control of strain both during film fabrication and during subsequent cooling, including the effect of phase transformations. One of the distinguishing features of this effort will be the use of various in-situ techniques for characterizing film growth, with a particular focus on understanding the initial stages of film growth and interaction with the substrate. Work will focus on $Ba_xSr_{1-x}TiO_3$ (BST), $Pb(Zr_xTi_{1-x})O_3$ (PZT), and $KNbO_3$ (KNO) as important model perovskites.

Objective 2: Determine the relationship between the critical electrical properties (dielectric and ferroelectric) and the film microstructure, strain, and perovskite/substrate interfacial interactions. This effort will focus on elucidating the ferroelectric behavior for nanoscale systems, such as domain dynamics in constrained systems, and the issues that are critical for integrating perovskite films (BST and PZT) into silicon based micro and nanosystems.

One of the key strengths of this program is that it brings together many of the leading U.S. programs in perovskite film growth, characterization, integration and modeling. Given the complexity of the problems, it is critical to have such an interdisciplinary effort that coordinates the expertise and resources at four National Laboratories, Five Universities, and industrial partners. While there are already substantive collaborations among some members of our team, the main programmatic value of the project will be to couple independent, parallel and complementary efforts already supported by the Basic Energy Sciences Program and other DOE programs at the participating institutions.

The project consists of two tasks: (1) Controlled Growth of Perovskite Films on Silicon Substrates, and (2) Nanoscale Structure-Property Relationships of Perovskite Films.

Granular Flow and Kinetics

Participating Labs:	Ames Lab, ANL, LANL, SNL/NM
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The goal of this project is to develop constitutive relationships for the dynamic response of granular materials capturing the breadth of granular kinetics and flows in fundamental ways. The research is organized under two tasks:

1. Dynamic constitutive relations for granular flow. Improve continuum hydrodynamic and kinetic theory descriptions via statistical studies of granular assemblies with a large number of particles. In particular, the role of impulsive collisions and dissipative interparticle interations will be examined. Multiphase granular flows, chute flows, avalanches and electrically driven systems will be studied. Issues include avalanching, segregation, and cluster formation.
2. Low dimensions, constrained granular dynamics. Seek universal behavior between disparate systems, such as granular systems with magnetic, electric, and

capillary forces, tethers and chain-like constraints. A strategy for understanding general systems is to reduce dimensionality and add constraints – sometimes promoting new phenomena – leading to the important question of mapping behavior from 2D to 3D.

Synthesis and Processing of Carbon-Based Nanostructured Materials

Participating Labs:	ANL, LBNL, ORNL, SNL/NM, N. Carolina State Univ. and Northwestern Univ.	
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The objective of this project is to advance the science and technology of carbon-based materials that will lead to the development of a new generation of MEMS and NEMS devices. The Project's activities are focused on: a) investigation of fundamental processes and phenomena related to carbon materials in the various forms of micro- and nanocrystalline diamond, diamond-like carbon, nanofibers and nanotubes, and b) development of MEMS and NEMS devices and their implementation to enable the exploration of fundamental processes in carbon materials at the micro- and nanoscales. The Project thus focuses not only on Nanoscience, but also on the development of the microscale and nanoscale instrumentation needed to conduct that science. The overall approach of the Project is to effectively couple existing programs in carbon-based systems in order to enable collaborative interactions that would otherwise not occur. In addition, the proposed Project's research focus is directly related to a major area of new emphasis in DOE-BES, i.e., the National Nanotechnology Initiative, and also fits with DOE's programmatic objectives of supporting major Centers of Nanoscience Research at several National Laboratories.

The Project is organized into two tasks: (1) Synthesis, processing and fundamental mechanical and tribological properties of nanoscale carbon-based materials, and (2) fundamental transport processes in nanoscale carbon-based materials.